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3-(4-*tert*-Butylphenyl)-1-(4-fluorophenyl)-3-hydroxyprop-2-en-1-one

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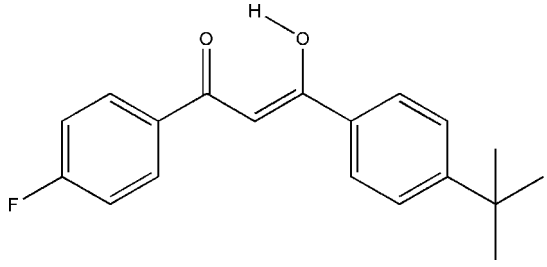
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.002 Å; R factor = 0.050; wR factor = 0.131; data-to-parameter ratio = 15.1.

The title molecule, $C_{19}H_{19}FO_2$, exits in the enol form with a dihedral angle of 33.06 (8)° between the two benzene rings. The molecular conformation is stabilized in part by an intramolecular O—H···O hydrogen bond.

Related literature

For background information on 1,3-diketones, see: Baskar & Roesky (2005); Bassett *et al.* (2004); Bertolasi *et al.* (1991); Jang *et al.* (2006); Soldatov *et al.* (2003); Vila *et al.* (1991).



Experimental

Crystal data

$C_{19}H_{19}FO_2$
M_r = 298.34
Monoclinic, $P2_1/n$
a = 9.8349 (12) Å
b = 10.0163 (13) Å
c = 16.232 (2) Å
β = 97.788 (2)°
V = 1584.3 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 (2) K
0.20 × 0.10 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.993, T_{max} = 0.995
12039 measured reflections
3099 independent reflections
2199 reflections with $I > 2\sigma(I)$
R_{int} = 0.074

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.131
S = 1.00
3099 reflections
205 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2A···O1	1.16 (2)	1.38 (2)	2.4720 (16)	154 (2)

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2743).

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supplementary materials

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3-(4-*tert*-Butylphenyl)-1-(4-fluorophenyl)-3-hydroxyprop-2-en-1-one

C. Zheng, D. Wang and L. Fan

Comment

1,3-Diketones are interesting due to their enolic tautomeric forms and their ability to form strong intermolecular or intramolecular hydrogen bonds (Bertolasi *et al.*, 1991; Vila *et al.*, 1991). They are used widely in the chemistry of metallo-complexes (Baskar *et al.*, 2005; Bassett *et al.*, 2004; Jang *et al.*, 2006; Soldatov *et al.*, 2003). The title compound (I) (Fig. 1), is in the enol form stabilized by an intramolecular O-H···O hydrogen bond (see Table 1).

Experimental

1-(4-fluorophenyl)ethanone (1.38 g, 0.01 mol), methyl 4-*tert*-butylbenzoate (1.92 g, 0.01 mol), $NaNH_2$ (0.78 g, 0.02 mol) and dry ether (60 ml) were placed into round bottom flask. The mixture was stirred for 6 h at room temperature under a blanket of nitrogen, acidified with dilute hydrochloric acid, and stirring was continued until all solids dissolved. The ether layer was separated and washed with saturated $NaHCO_3$ solution, dried over anhydrous Na_2SO_4 and was removed by evaporation. The residual solid was recrystallized from ethanol solution to give the title compound (I) (yield 1.78 g, 59.6%, m.p. 388 K). Crystals suitable for X-ray diffraction were grown by slow evaporation of a $CHCl_3$—EtOH (1:4) solution of the title compound at room temperature.

Refinement

H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.93 to 0.96 Å, and with U_{iso}(H) = 1.2 U_{eq}(C). The H atom of the hydroxyl group was located in a difference Fourier map and its position was refined freely, with U_{iso}(H) = 1.5 U_{iso}(O).

Figures

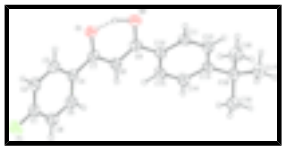


Fig. 1. The molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level. The dashed line indicates a intramolecular hydrogen bond.

3-(4-*tert*-Butylphenyl)-1-(4-fluorophenyl)-3-hydroxyprop-2-en-1-one

Crystal data

$C_{19}H_{19}FO_2$	F_{000} = 632
M_r = 298.34	D_x = 1.251 Mg m^{-3}
Monoclinic, $P2_1/n$	Melting point: 388 K
Hall symbol: -P 2yn	Mo $K\alpha$ radiation

	λ = 0.71073 Å
a = 9.8349 (12) Å	Cell parameters from 3223 reflections
b = 10.0163 (13) Å	θ = 2.3–22.9º
c = 16.232 (2) Å	μ = 0.09 mm^{-1}
β = 97.788 (2)º	T = 298 (2) K
V = 1584.3 (3) Å^3	Block, colorless
Z = 4	0.20 × 0.10 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer	3099 independent reflections
Radiation source: fine-focus sealed tube	2199 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.074
T = 298(2) K	θ_{max} = 26.0º
φ and ω scans	θ_{min} = 2.3º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -11 \rightarrow 12$
T_{min} = 0.993, T_{max} = 0.995	$k = -12 \rightarrow 12$
12039 measured reflections	$l = -19 \rightarrow 19$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.050	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.131	$w = 1/[\sigma^2(F_o^2) + (0.07P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.00	$(\Delta/\sigma)_{max}$ = 0.001
3099 reflections	$\Delta\rho_{max}$ = 0.17 e Å^{-3}
205 parameters	$\Delta\rho_{min}$ = −0.18 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.12996 (18)	0.09274 (19)	−0.07276 (10)	0.0599 (5)
C2	0.0803 (2)	0.2198 (2)	−0.08119 (10)	0.0666 (5)
H2	0.0522	0.2559	−0.1335	0.080*
C3	0.07296 (18)	0.29335 (17)	−0.01033 (9)	0.0587 (5)
H3	0.0401	0.3805	−0.0150	0.070*
C4	0.11376 (15)	0.23969 (16)	0.06796 (9)	0.0457 (4)
C5	0.16498 (16)	0.11083 (17)	0.07303 (9)	0.0545 (4)
H5	0.1943	0.0741	0.1250	0.065*
C6	0.17340 (17)	0.03602 (18)	0.00290 (10)	0.0596 (5)
H6	0.2076	−0.0506	0.0068	0.071*
C7	0.09992 (16)	0.32242 (16)	0.14225 (9)	0.0491 (4)
C8	0.11727 (16)	0.27023 (16)	0.22333 (9)	0.0499 (4)
H8	0.1464	0.1824	0.2321	0.060*
C9	0.09179 (16)	0.34703 (16)	0.29012 (9)	0.0498 (4)
C10	0.09963 (16)	0.29479 (16)	0.37555 (9)	0.0475 (4)
C11	0.01481 (18)	0.34617 (16)	0.42948 (10)	0.0561 (4)
H11	−0.0459	0.4148	0.4118	0.067*
C12	0.01961 (17)	0.29659 (17)	0.50883 (10)	0.0565 (4)
H12	−0.0396	0.3319	0.5432	0.068*
C13	0.10956 (15)	0.19580 (15)	0.53959 (9)	0.0464 (4)
C14	0.19521 (17)	0.14742 (17)	0.48502 (9)	0.0557 (4)
H14	0.2580	0.0808	0.5032	0.067*
C15	0.19034 (17)	0.19472 (17)	0.40495 (9)	0.0541 (4)
H15	0.2488	0.1589	0.3702	0.065*
C16	0.11634 (16)	0.14446 (16)	0.62880 (9)	0.0512 (4)
C17	−0.02548 (19)	0.1488 (2)	0.65807 (11)	0.0744 (6)
H17A	−0.0544	0.2400	0.6614	0.112*
H17B	−0.0205	0.1080	0.7119	0.112*
H17C	−0.0903	0.1012	0.6193	0.112*
C18	0.2134 (2)	0.2360 (2)	0.68505 (10)	0.0774 (6)
H18A	0.3020	0.2364	0.6664	0.116*
H18B	0.2221	0.2039	0.7412	0.116*
H18C	0.1770	0.3250	0.6827	0.116*
C19	0.1691 (2)	0.00150 (18)	0.63681 (12)	0.0791 (6)
H19A	0.1140	−0.0541	0.5973	0.119*
H19B	0.1639	−0.0305	0.6920	0.119*
H19C	0.2628	−0.0010	0.6262	0.119*
F1	0.13561 (14)	0.01881 (12)	−0.14199 (6)	0.0933 (4)
O1	0.06597 (13)	0.44469 (12)	0.12968 (7)	0.0671 (4)
O2	0.05431 (14)	0.47163 (12)	0.27994 (8)	0.0720 (4)
H2A	0.050 (2)	0.485 (2)	0.2088 (15)	0.108*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0655 (12)	0.0679 (12)	0.0478 (9)	0.0042 (9)	0.0136 (8)	−0.0004 (8)
C2	0.0872 (14)	0.0695 (13)	0.0436 (9)	0.0131 (10)	0.0110 (8)	0.0131 (8)
C3	0.0709 (12)	0.0531 (10)	0.0526 (10)	0.0069 (9)	0.0105 (8)	0.0105 (8)
C4	0.0383 (9)	0.0509 (10)	0.0480 (9)	−0.0008 (7)	0.0060 (6)	0.0057 (7)
C5	0.0546 (10)	0.0619 (11)	0.0458 (9)	0.0075 (8)	0.0026 (7)	0.0083 (8)
C6	0.0628 (12)	0.0584 (11)	0.0574 (10)	0.0130 (9)	0.0080 (8)	0.0037 (8)
C7	0.0445 (9)	0.0480 (10)	0.0540 (9)	−0.0026 (7)	0.0035 (7)	0.0054 (7)
C8	0.0547 (10)	0.0466 (10)	0.0475 (9)	0.0040 (8)	0.0040 (7)	0.0024 (7)
C9	0.0493 (10)	0.0455 (10)	0.0525 (9)	−0.0028 (7)	−0.0003 (7)	−0.0013 (7)
C10	0.0484 (9)	0.0456 (9)	0.0468 (8)	−0.0007 (7)	0.0004 (7)	−0.0062 (7)
C11	0.0625 (11)	0.0490 (10)	0.0560 (10)	0.0152 (8)	0.0049 (8)	0.0000 (7)
C12	0.0612 (11)	0.0559 (11)	0.0537 (10)	0.0124 (9)	0.0128 (8)	−0.0052 (8)
C13	0.0465 (9)	0.0443 (9)	0.0475 (8)	−0.0021 (7)	0.0028 (7)	−0.0069 (7)
C14	0.0547 (10)	0.0603 (11)	0.0507 (9)	0.0163 (8)	0.0017 (7)	0.0021 (7)
C15	0.0531 (10)	0.0615 (11)	0.0480 (9)	0.0132 (8)	0.0075 (7)	−0.0049 (7)
C16	0.0502 (10)	0.0554 (10)	0.0471 (9)	−0.0006 (8)	0.0029 (7)	−0.0021 (7)
C17	0.0699 (13)	0.0938 (15)	0.0614 (11)	−0.0013 (11)	0.0153 (9)	0.0105 (10)
C18	0.0857 (14)	0.0914 (15)	0.0515 (10)	−0.0224 (12)	−0.0039 (9)	−0.0023 (9)
C19	0.1093 (17)	0.0651 (13)	0.0644 (12)	0.0161 (12)	0.0167 (11)	0.0115 (9)
F1	0.1407 (12)	0.0884 (9)	0.0527 (6)	0.0260 (7)	0.0201 (6)	−0.0074 (5)
O1	0.0956 (10)	0.0484 (7)	0.0566 (7)	0.0054 (7)	0.0083 (6)	0.0085 (5)
O2	0.1083 (11)	0.0459 (7)	0.0598 (8)	0.0109 (7)	0.0044 (7)	−0.0007 (5)

Geometric parameters (Å, °)

C1—F1	1.3532 (19)	C11—H11	0.9300
C1—C2	1.364 (3)	C12—C13	1.390 (2)
C1—C6	1.368 (2)	C12—H12	0.9300
C2—C3	1.376 (2)	C13—C14	1.390 (2)
C2—H2	0.9300	C13—C16	1.530 (2)
C3—C4	1.388 (2)	C14—C15	1.378 (2)
C3—H3	0.9300	C14—H14	0.9300
C4—C5	1.384 (2)	C15—H15	0.9300
C4—C7	1.485 (2)	C16—C19	1.523 (2)
C5—C6	1.375 (2)	C16—C18	1.533 (2)
C5—H5	0.9300	C16—C17	1.534 (2)
C6—H6	0.9300	C17—H17A	0.9600
C7—O1	1.2784 (19)	C17—H17B	0.9600
C7—C8	1.405 (2)	C17—H17C	0.9600
C8—C9	1.380 (2)	C18—H18A	0.9600
C8—H8	0.9300	C18—H18B	0.9600
C9—O2	1.3054 (19)	C18—H18C	0.9600
C9—C10	1.474 (2)	C19—H19A	0.9600
C10—C15	1.383 (2)	C19—H19B	0.9600
C10—C11	1.387 (2)	C19—H19C	0.9600

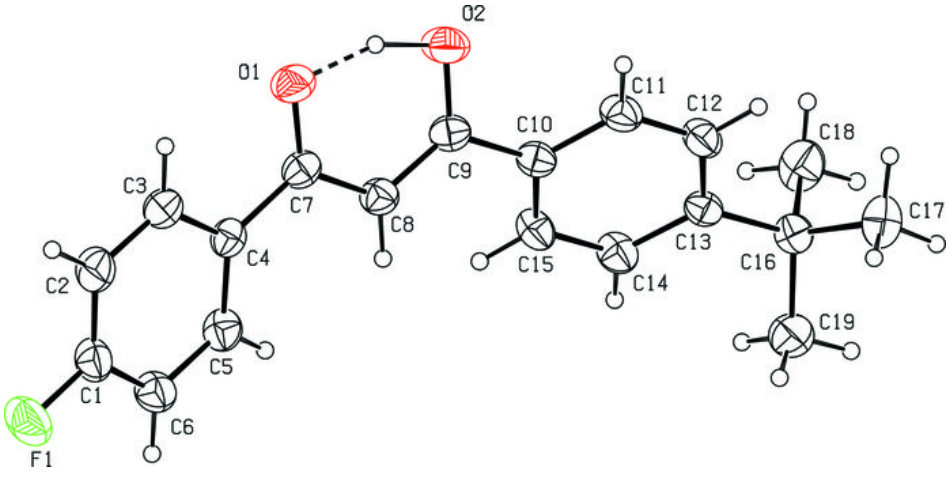
C11—C12	1.375 (2)	O2—H2A	1.16 (2)
F1—C1—C2	118.81 (15)	C14—C13—C12	115.83 (14)
F1—C1—C6	118.39 (16)	C14—C13—C16	122.26 (14)
C2—C1—C6	122.81 (16)	C12—C13—C16	121.89 (14)
C1—C2—C3	118.32 (15)	C15—C14—C13	122.32 (15)
C1—C2—H2	120.8	C15—C14—H14	118.8
C3—C2—H2	120.8	C13—C14—H14	118.8
C2—C3—C4	121.11 (16)	C14—C15—C10	120.86 (15)
C2—C3—H3	119.4	C14—C15—H15	119.6
C4—C3—H3	119.4	C10—C15—H15	119.6
C5—C4—C3	118.25 (14)	C19—C16—C13	111.57 (14)
C5—C4—C7	123.03 (13)	C19—C16—C18	109.51 (15)
C3—C4—C7	118.72 (14)	C13—C16—C18	107.85 (13)
C6—C5—C4	121.43 (14)	C19—C16—C17	108.31 (15)
C6—C5—H5	119.3	C13—C16—C17	111.03 (13)
C4—C5—H5	119.3	C18—C16—C17	108.51 (15)
C1—C6—C5	118.07 (16)	C16—C17—H17A	109.5
C1—C6—H6	121.0	C16—C17—H17B	109.5
C5—C6—H6	121.0	H17A—C17—H17B	109.5
O1—C7—C8	120.13 (14)	C16—C17—H17C	109.5
O1—C7—C4	117.12 (13)	H17A—C17—H17C	109.5
C8—C7—C4	122.71 (14)	H17B—C17—H17C	109.5
C9—C8—C7	121.11 (15)	C16—C18—H18A	109.5
C9—C8—H8	119.4	C16—C18—H18B	109.5
C7—C8—H8	119.4	H18A—C18—H18B	109.5
O2—C9—C8	120.78 (14)	C16—C18—H18C	109.5
O2—C9—C10	115.86 (14)	H18A—C18—H18C	109.5
C8—C9—C10	123.32 (15)	H18B—C18—H18C	109.5
C15—C10—C11	117.77 (15)	C16—C19—H19A	109.5
C15—C10—C9	122.06 (14)	C16—C19—H19B	109.5
C11—C10—C9	120.17 (15)	H19A—C19—H19B	109.5
C12—C11—C10	120.64 (15)	C16—C19—H19C	109.5
C12—C11—H11	119.7	H19A—C19—H19C	109.5
C10—C11—H11	119.7	H19B—C19—H19C	109.5
C11—C12—C13	122.56 (15)	C7—O1—H2A	101.2 (10)
C11—C12—H12	118.7	C7—O1—H2A	101.2 (10)
C13—C12—H12	118.7	C9—O2—H2A	102.1 (11)
F1—C1—C2—C3	178.96 (17)	O2—C9—C10—C11	29.4 (2)
C6—C1—C2—C3	−0.5 (3)	C8—C9—C10—C11	−148.40 (16)
C1—C2—C3—C4	−0.5 (3)	C15—C10—C11—C12	−1.3 (3)
C2—C3—C4—C5	1.3 (3)	C9—C10—C11—C12	178.87 (15)
C2—C3—C4—C7	−178.35 (16)	C10—C11—C12—C13	1.2 (3)
C3—C4—C5—C6	−1.2 (2)	C11—C12—C13—C14	0.0 (3)
C7—C4—C5—C6	178.49 (15)	C11—C12—C13—C16	178.28 (15)
F1—C1—C6—C5	−178.81 (15)	C12—C13—C14—C15	−0.9 (3)
C2—C1—C6—C5	0.6 (3)	C16—C13—C14—C15	−179.20 (15)
C4—C5—C6—C1	0.2 (3)	C13—C14—C15—C10	0.7 (3)
C5—C4—C7—O1	172.32 (15)	C11—C10—C15—C14	0.4 (3)

C3—C4—C7—O1	−8.0 (2)	C9—C10—C15—C14	−179.79 (15)
C5—C4—C7—C8	−10.2 (2)	C14—C13—C16—C19	−27.3 (2)
C3—C4—C7—C8	169.45 (15)	C12—C13—C16—C19	154.50 (16)
O1—C7—C8—C9	3.2 (2)	C14—C13—C16—C18	93.01 (19)
C4—C7—C8—C9	−174.20 (14)	C12—C13—C16—C18	−85.19 (19)
C7—C8—C9—O2	−1.8 (2)	C14—C13—C16—C17	−148.23 (16)
C7—C8—C9—C10	175.89 (14)	C12—C13—C16—C17	33.6 (2)
O2—C9—C10—C15	−150.37 (16)	C8—C7—O1—H2A	−3.3 (9)
C8—C9—C10—C15	31.8 (2)	C4—C7—O1—H2A	174.2 (9)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2A···O1	1.16 (2)	1.38 (2)	2.4720 (16)	154 (2)

Fig. 1


O2
O1
C11
C12
C10
C18
C3
C9
C7
C8
C17
C4
C13
C2
C15
C16
C14
C19
C5
C1
C6
F1